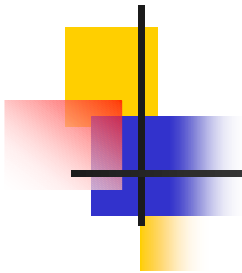


“TOXNET on the Web”

Toxicology and Environmental Health Information
from the National Library of Medicine (NLM)
and Other Sites



Presented by

NLM's Toxicology and Environmental Health Information Program

part of the Division of Specialized Information Services

Contact:

Toxicology and Environmental Health Information Program

Division of Specialized Information Services

National Library of Medicine

Suite 510, MSC 5467

6707 Democracy Blvd.

Bethesda, MD 20892-5467

301-496-1131

301-480-3537 (FAX)

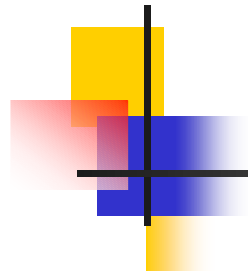
<http://sis.nlm.nih.gov/>

tehip@tehl.nlm.nih.gov



Class Schedule

Part I	Overview of NLM Tox Resources	9:00 - 9:30
Part II	TOXNET Overview, HSDB & Related Files	9:30 - 10:30
	<i>Break</i>	10:30 - 10:45
Part III	TOXLINE and Related Files	10:45 - 11:30
	<u>Practicum</u>	11:30 - 12:15
	<i>Lunch</i>	12:15 - 1:30
Part IV	TRI and other Specialty Files	1:30 - 2:15
Part V	Non-NLM Resources	2:15 - 3:00
	<i>Break</i>	3:00 - 3:15
Part VI	ChemIDplus	3:15 - 3:45
	<u>Practicum</u>	3:45 - 4:30



Part I

An Overview of Toxicology and Environmental Health Information Resources at the National Library of Medicine



Toxicology and Environmental Health Information Program (TEHIP)

Background

- Poisons recognized throughout time.
- Harvey W. Wiley's Poison Squad – 1903
- The Jungle (1906) Upton Sinclair – lack of hygiene in the meat-packing industry
- Food and Drugs Act (1906) – prohibited adulterated or misbranded items
- Federal Food, Drug and Cosmetic Act (1938) – enhanced safety requirements for drugs
- Drug Amendments (1962) – effectiveness required for drugs
- Silent Spring (1962) Rachel Carson – sparked public awareness about hazards of synthetic chemicals
- President's Science Advisory Committee (1966) – “Report on the Handling of Toxicological Information”
- TEHIP Created (1967)
- Situated within NLM's Division of Specialized Information Services



TEHIP Mission

- Provide selected core toxicology and environmental health information resources and services
- Facilitate access to national and international toxicology and environmental health information resources
- Strengthen the information infrastructure of toxicology and environmental health

So...TEHIP

- Builds and/or makes available free online Web-based databases
- Creates other Web-based resources
- Collaborates with government agencies and others
- Is active in public training and outreach



TEHIP Databases

- TOXNET System of Databases (including ChemID*plus* and Specialty Databases)
- DIRLINE (directory of organizations)

Additional TEHIP Resources

- Special Topic Guides – arsenic, biological & chemical warfare agents, etc.
- Publications (including Glossary of Terms Used in Toxicology)
- Toxicology Tutor

Other Relevant NLM Information

- PubMed/MEDLINE
- MEDLINE*plus* (consumer health, includes drug information)
- Clinical Trials
- NLM Gateway – Multi-File Searching – Planned to go across all NLM Files



About

The Specialized Information Services (SIS) Division of the National Library of Medicine (NLM) is responsible for information resources and services in toxicology, environmental health, chemistry, HIV/AIDS, and specialized topics in minority health.



Toxicology & Environmental Health

Databases and other resources related to toxicology and environmental health. Features [TOXNET](#), **Improved**



Chemical Information

Databases and other resources designed to help you search for information by chemical name or structure. Features [ChemDp/us](#).



HIV / AIDS

Links to journal literature, clinical trials and treatment information, meeting abstracts, and other scientific and consumer-related resources.



Directory of Health Organizations

Features [DIRLINE](#) **improved** and [Health Hotlines](#).

More to Explore

[News](#)

[Outreach Activities](#)

Other NLM Resources

[NLM Gateway](#) search multiple NLM databases

[MEDLINE/PubMed](#)

search journal literature

[LOCATORplus](#) books, journals, audiovisuals

[Staff Directory](#)

[Site Map and Search](#)

Special Topics

[Arsenic](#) **NEW**

TOXNET & DIRLINE

NEW

• Streamlined search interface

• Search all TOXNET databases at once



Toxicology and Environmental Health

TOXNET

Databases in toxicology and environmental health.

[TOXLINE](#) [HSDB](#) [ChemIDplus](#)
[DART](#) [TRI](#) [IRIS](#)
[GENETOX](#) [CCRIS](#)

Special Topics

Evaluated links to Internet resources on current issues such as [arsenic](#) or [chemical warfare](#).

Haz-Map

Database on hazardous chemicals and occupational diseases.

AltBib

References about alternatives to the use of live animals in biomedical research and testing.

Toxicology Tutor

Three self-guided tutorials on toxicology.

News and Events

Links to news items on the web site, [outreach activities](#) and a [calendar of events](#).

Consumer Health

[MEDLINEplus](#)

[Poisoning, Toxicology and Environmental Health](#)

[DIRLINE](#)

Over 10,000 health organizations.

[Health Hotlines](#)

Toll-free numbers to 300 organizations.

MEDLINE/PubMed

References from more than 4,600 biomedical journals, including the [Toxicology Subset](#).

Other Resources

[Chemical Information](#)
[Selected Toxicology Links](#)
[Reference Material](#)

Bibliographies, glossary, reports.

[Database descriptions](#)

[Lecture guides](#)

[Locatorplus](#)

The NLM catalog of books, journals, and audiovisuals.

[NLM Gateway](#)

Search multiple retrieval systems at NLM.



Directory of Health Organizations Online

► [Directory of Health Organizations](#) ►
DIRLINE

[Search DIRLINE](#)

[Other NLM Resources](#)

drinking water

[Search](#)

[Clear](#)

Search:

☒ all of the words ☐ any of the words ☐ exact phrase

Fields: (if none checked, all fields will be searched.)

☐ Organization name or acronym

☐ MeSH Headings/Keywords

Select records containing:

☐ Only organizations with toll-free numbers

☐ Only organizations with services for the hearing impaired

[Search](#)

[Browse the Index](#)

[Health Hotlines](#)

[MEDLINEplus](#)

[PubMed](#)

[NLM Gateway](#)

[Locatorplus](#)

[Support Page](#)

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[Disclaimer](#)

[Suggestion Form](#)



DIRLINE Search Results

[Directory of Health Organizations](#)

[DIRLINE](#)

[Save
Checked Items](#)

[Sort](#)

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[SIS
Home](#)

[MEDLINEplus
Home](#)

drinking water

[Search](#)

[Clear](#)

Items 1 through 20 of 49

Pages: [1](#) [2](#) [3](#) [▶](#)

Organization Names are sorted in *relevancy ranked* order.

Select Record	Organization Name
1 <input type="checkbox"/>	Drinking Water Program - Massachusetts Department of Environmental Protection
2 <input type="checkbox"/>	National Drinking Water Clearinghouse - Environmental Services and Training Division - West Virginia University (NDWC)
3 <input type="checkbox"/>	Office of Water Quality - Indiana Department of Environmental Management
4 <input type="checkbox"/>	U.S. Environmental Protection Agency - Office of Research and Development - National Risk Management Research Laboratory - Water Supply and Water Resources Division
5 <input type="checkbox"/>	Office of Drinking Water Quality - Rhode Island Department of Health
6 <input type="checkbox"/>	American Water Works Association (AWWA)
7 <input type="checkbox"/>	Office of Water, U.S. Environmental Protection Agency (OW)
8 <input type="checkbox"/>	WATERNET - American Water Works Association - Information Services
9 <input type="checkbox"/>	Drinking Water Program - Drinking Water and Environmental Management Division - California Department of Health Services
10 <input type="checkbox"/>	Water Environment Federation (WEF)
11 <input type="checkbox"/>	Clean Water Action (CWA)
12 <input type="checkbox"/>	Nevada Department of Human Resources - Division of Health - Bureau of Health Protection Services
13 <input type="checkbox"/>	Kentucky Natural Resources and Environmental Protection Cabinet - Department for Environmental Protection - Division of Water
14 <input type="checkbox"/>	Maine Department of Human Services - Division of Health Engineering (MEDHE)
15 <input type="checkbox"/>	Environmental Health Services - Fulton County Board of Health
16 <input type="checkbox"/>	International Office For Water - Office International de L'Eau
17 <input type="checkbox"/>	American Water Resources Association (AWRA)
18 <input type="checkbox"/>	New England Water Works Association (NEWWA)

Poisoning, Toxicology, Environmental Health Topics

- [Air Pollution](#)
- [Anthrax](#)
- [Arsenic](#)
- [Asbestos/Asbestosis](#)
- [Biological and Chemical Weapons](#)
- Bioterrorism see [Biological and Chemical Weapons](#)
- Campylobacter see [Food Contamination/Poisoning](#)
- [Carbon Monoxide Poisoning](#)
- Cell Phones see [Electromagnetic Fields](#)
- Chemical Weapons see [Biological and Chemical Weapons](#)
- Cleaning Products see [Household Poisons](#)
- [Drinking Water](#)
- EMF see [Electromagnetic Fields](#)
- [Electromagnetic Fields](#)
- [Environmental Health](#)
- Environmental Tobacco Smoke see [Secondhand Smoke](#)
- [Food Contamination/Poisoning](#)
- [Food Safety](#)
- Fungicides see [Pesticides](#)
- Germ Warfare see [Biological and Chemical Weapons](#)
- Hazardous Waste see [Environmental Health](#)
- Herbicides see [Pesticides](#)
- [Household Poisons](#)
- [Indoor Air Pollution](#)
- Insecticides see [Pesticides](#)
- [Lead Poisoning](#)
- [Mercury](#)
- Mesothelioma see [Asbestos/Asbestosis](#)
- [Molds](#)
- [Noise](#)
- Norwalk Virus Infections see [Food Contamination/Poisoning](#)
- [Ozone](#)
- Passive Smoking see [Secondhand Smoke](#)
- [Pesticides](#)
- Plague see [Biological and Chemical Weapons](#)
- [Poisoning](#)
- Poisons in the Home see [Household Poisons](#)
- [Radiation Exposure](#)
- [Radon](#)
- Rodenticides see [Pesticides](#)
- [Secondhand Smoke](#)
- [Smallpox](#)
- Smoking, Passive see [Secondhand Smoke](#)
- Tularemia see [Biological and Chemical Weapons](#)
- Water see [Drinking Water](#)
- Yersinia see [Food Contamination/Poisoning](#)

[Browse](#) : [By Condition](#) : [By Disease Heading](#) : [Injuries, Poisonings, and Occupational Diseases](#) : **Disorders of Environmental Origin**

☐ Show all trials, including those no longer recruiting patients.

Click on title to see details. Or, select multiple checkboxes and press "Display Selected Studies" at bottom of page.

150 studies were found. Here are studies 1 to 50. [Next 50](#)

1. ☐ **Recruiting** [Reducing Pesticide Exposure in Minority Families](#)
Condition: Disorders of Environmental Origin
2. ☐ **Recruiting** [Does Lead Burden alter Neuropsychological Development?](#)
Condition: Lead Poisoning
3. ☐ **Recruiting** [Cocaine Effects in Humans: Physiology and Behavior](#)
Condition: Cocaine-Related Disorders
4. ☐ **Not yet recruiting** [Pharmacological Modulation of Cocaine Effects](#)
Condition: Cocaine-Related Disorders
5. ☐ **Recruiting** [IV Cocaine Abuse: A Laboratory Model](#)
Condition: Cocaine-Related Disorders
6. ☐ **Recruiting** [Combined Buprenorphine and Behavioral Tx w/out contingent reinforcement](#)
Conditions: Cocaine-Related Disorders; Opioid-Related Disorders
7. ☐ **Recruiting** [Flupenthixol Decanoate in Methamphetamine Smoking](#)
Condition: Substance-Related Disorders
8. ☐ **Recruiting** [Evaluation of Opioid Antagonist Activity in Humans](#)
Condition: Opioid-Related Disorders
9. ☐ **Recruiting** [Evaluation of a Desipramine Ceiling in Cocaine Abuse](#)
Conditions: Substance-Related Disorders; Cocaine-Related Disorders
10. ☐ **Not yet recruiting** [Risperidone Treatment in Dually-Diagnosed Individuals](#)
Condition: Cocaine-Related Disorders
11. ☐ **Recruiting** [Cocaine Abuse and Attention Deficit Disorder](#)
Condition: Cocaine-Related Disorders
12. ☐ **Recruiting** [Pergolide Treatment for Substance Abusers](#)
Conditions: Substance-Related Disorders; Cocaine-Related Disorders



Gateway

your entrance to the
knowledge resources of the
National Library of Medicine

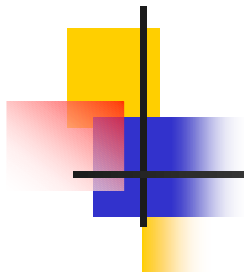
[Search](#)[Clear
Search](#)[Find Terms](#)[Limits](#)[Results](#)[History](#)[Locker](#)[Preferences](#)[New Search](#)

Results Summary

[History](#)[Overview](#)[What's New](#)[Help](#)[FAQ](#)[Other NLM
Resources](#)[Ordering Info.](#)[Clinical Alerts](#)[ClinicalTrials.gov](#)[HSTAT](#)[LOCATORplus](#)[MEDLINEplus](#)[PubMed](#)[TOXNET](#)

Category	Items Found	Actions	
Journal Citations	1882	Display Results	Details of Search
Books / Serials / AVs	23	Display Results	Details of Search
Consumer Health	10	Display Results	Details of Search
Meeting Abstracts	1	Display Results	Details of Search
Other Collections	2	Display Results	Details of Search
Total	1918		

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Part II

TOXNET Overview, HSDB, & Related Files



What is TOXNET?

- A free web-based system of databases on toxicology, environmental health, hazardous chemicals, toxic releases, chemical nomenclature, and specialty areas such as occupational health and consumer products
- A product of NLM's Toxicology and Environmental Health Information Program
- Toxicology Data (one record per chemical)– HSDB, IRIS, CCRIS, GENE-TOX (can also search any combination of these files with “Multi-Databases” interface)
- Toxicology Literature (bibliographic references) – TOXLINE, DART/ETIC
- Toxic Releases (of chemicals to the environment) – TRI
- Chemical Identification/Nomenclature – ChemIDplus
- Specialty Databases – HazMap, Consumer Products
- User Support – tehip@the.nlm.nih.gov or click on “Contact TOXNET”

Where is TOXNET?

toxnet.nlm.nih.gov



TOXNET

► [Tox. & Env. Health](#) ► [TOXNET](#)

Welcome to TOXNET, a cluster of databases on toxicology, hazardous chemicals, and related areas.

Databases

HSDB	i
IRIS	i
GENE-TOX	i
CCRIS	i
Multi-Databases	i
TOXLINE	i
DART/ETIC	i
TRI	i
ChemIDplus	i

Search All Databases

Other NLM Resources

[DIRLINE](#)
[Tox Weblinks](#)
[MEDLINEplus](#)
[Tox/Env. Health subset](#)
[PubMed](#)
[NLM Gateway](#)
[Locatorplus](#)

Support Pages

[Help](#)
[Database Descriptions](#)
[News](#)



TOXNET

► [Tox. & Env. Health](#) ► [TOXNET](#)

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GENE-TOX	i
CCRIS	i
Multi-Databases	i
TOXLINE	i
DART/ETIC	i
TRI	i
ChemIDplus	i

Search All Databases

Other NLM Resources

[DRLINE](#)
[Tox Weblinks](#)
[MEDLINEplus](#)
[Tox/Env. Health subset](#)
[PubMed](#)
[NLM Gateway](#)
[Locatorplus](#)

Search Results:

Database	Records found i
TOXLINE Special	3558
DART Special	69
HSDB	51
IRIS	1
GENETOX	1
CCRIS	1
TRI	6
CHEMIDplus	1

Support Pages

[Help](#)
[Database Descriptions](#)
[News](#)



Toxicology Data Files - Content

Hazardous Substances Data Bank (HSDB) – from NLM

4637 Chemical Records

Human Health Effects

Emergency Medical Treatment

Animal Toxicity Studies

Metabolism/Pharmacokinetics

Pharmacology

Environmental Fate/Exposure

Environmental Standards & Regulations

Chemical/Physical Properties

Chemical Safety & Handling

Occupational Exposure Standards

Manufacturing and Use

Laboratory Methods

Special References

Synonyms and Identifiers



More about HSDB

- Factual Data Bank/Online Handbook
- Peer-Reviewed – Scientific Review Panel
- Review Status Tags – Peer Reviewed, QC Reviewed, Unreviewed
- Fully Referenced
- Data – Excerpted from books, government documents, technical reports, selected primary literature, databases. Some data compiled expressly for HSDB.



Toxicology Data Files - Content

Chemical Carcinogenesis Research Information System (CCRIS) – from the National Cancer Institute (NCI) 8837 Chemical Records

Carcinogenicity Studies

Tumor Inhibition Studies

Tumor Promotion Studies

Mutagenicity Studies

e.g. Carcinogenicity Studies Data Structure – species, route, tumor site/type of lesion, results, reference



Toxicology Data Files - Content

GENE-TOX

from the U.S. Environmental Protection Agency (EPA)

3200 Chemical Records

Note: GENE-TOX not updated since January 2000

Mutagenicity Studies

Data Structure – assay type, assay code, results, panel report, reference



Toxicology Data Files - Content

Integrated Risk Information System (IRIS)

from the U.S. Environmental Protection Agency (EPA)

538 Chemical Records

Noncarcinogenic Assessment – Oral (RfD)

Carcinogenic Assessment - Oral

Noncarcinogenic Assessment – Inhalation (RfC)

Carcinogenic Assessment -
Inhalation

- Contains EPA consensus scientific positions and quantitative values on cancer and non-cancer health effects that may result from lifetime oral or inhalation exposure to specific chemical substances in the environment
- Risk Assessment – Identification and quantification of risk. Function of toxicity and exposure
- Risk Assessment Process (National Academy of Sciences, 1983) – 1. Hazard identification, 2. Dose-Response assessment [IRIS], 3. Exposure assessment, 4. Risk Characterization



TOXNET Search Screen Options

- TOXNET Home Page Search
 - Single query box search
 - No limits
 - Gives quick counts of records retrieved and allows links to each database
 - Number of records retrieved in each database may vary from numbers attained by searching databases directly
- Database specific searches – interface varies according to type of database
- Multi-Databases search – interface for any combination of data files (i.e. HSDB, CCRIS, GENE-TOX, IRIS)

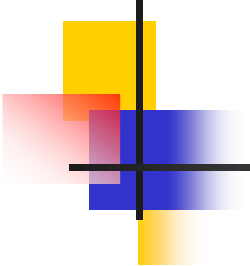


Search Page - Toxicology Data Files

- One Box Search for:
 - Chemicals – enter chemical names or CAS Registry numbers.
Let system add synonyms (default) or use exact terms entered.
 - Other Terms

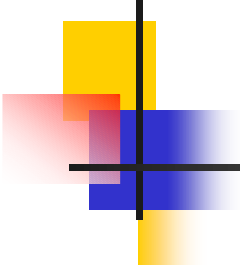
- Browse Index for:
 - All Words
 - Chemical name
 - CAS Registry Number

- Limits
 - For more precise searching – searching for terms within particular data fields (currently available for HSDB only, among the data file group.)



Search Results Page -Toxicology Data Files

- Displays chemical names and registry numbers of retrieved records
- Relevancy Ranked Display
- Select Record(s) of Interest
- View Details of Search Strategy
- Modify Search – Returns you to Search Page with query intact
- Begin a New Search – Returns you to Search Page with blank query box
- Or Search can be modified or begun anew directly on Results Page
- Sort Results – By substance name, ascending or descending sequence
- Save Checked Items, Display Checked Items
- View Search History and combine search statements
- Download – Entire Record(s) or Custom Format
- Browse Index
- Return to TOXNET Home



Selected Record Page - Toxicology Data Files

- Default display varies
 - Chemical Search – HSDB displays human health effects, other files display full record
 - Other Term(s) Search – Best Sections
- **Search Term(s) Highlighted in Red**
- Choose fields for display from Contents (expand, contract categories)
- Navigate – Next Item, Previous Item
- View Details of Search Strategy
- Modify Search – Returns you to Search Screen with query intact
- Begin a New Search – Returns you to Search Screen with blank query box
- Download – Entire Record(s) or Custom Format
- Browse Index
- Return to TOXNET Home
- Link to records for the same chemical in Other Files



Hazardous Substances Data Bank

► [Tox. & Env. Health](#) ► [TOXNET](#) ► [HSDB](#)

Databases

Hazardous Substances Data Bank	i
IRIS	i
GENE-TOX	i
CCRIS	i
Multi-Databases	i
TOXLINE	i
DART/ETIC	i
TRI	i
ChemIDplus	i
TOXNET Home	

Search HSDB

acetone

Search

Clear

For chemicals, add synonyms
and CAS numbers to search:

☒ Yes ☐ No

Limits

Browse the Index

Other NLM Resources

[DIRLINE](#)

[Tox Weblinks](#)

[MEDLINEplus](#)

[Tox/Env. Health subset](#)

[PubMed](#)

[NLM Gateway](#)

[Locatorplus](#)

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[Fact Sheet](#)

[Sample Record](#)

[HSDB Scientific Review
Panel](#)

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Customer Service: tehip@tehl.nlm.nih.gov

Last modified on May 8, 2002.



HSDB Search Results

[Tox. & Env. Health](#) ▶ [TOXNET](#) ▶ [HSDB](#)

Save
Checked Items

Sort

Details

History

Download

Modify Search

Basic Search

Browse Index

TOXNET Home

acetone

Search

Clear

Limits

For chemicals, add synonyms and CAS numbers to search: ☒ Yes ☐ No

Items 1 through 20 of 1846

Page 1 of 93. [Go](#) to page

Substance Names are sorted in [relevancy ranked](#) order.

Select
Record

Substance Name

The following is the primary record for the chemical. All of the query terms were found.

- 1 ☐ [ACETONE](#)
67-64-1

The following 1845 records contain one or more of the requested chemical name(s) and all of the query terms anywhere in the record.

- 2 ☐ [ACETONE CYANOHYDRIN](#)
75-86-5
- 3 ☐ [1-CHLORO-2-PROPANONE](#)
78-95-5
- 4 ☐ [ISOPROPANOL](#)
67-63-0
- 5 ☐ [1,1,1,3,3,3-HEXAFLUORO-2-PROPANONE](#)
684-16-2
- 6 ☐ [ACETONITRILE](#)
75-05-8
- 7 ☐ [ACETYL ACETONE](#)
123-54-6
- 8 ☐ [METHYL ETHYL KETONE](#)
78-93-3

Contents

Contract all categories

Expand all categories

Select

Clear

- ☐ [FULL RECORD](#)
- ☐ [Human Health Effects](#)
- ☐ [Emergency Medical Treatment](#)
- ☐ [Animal Toxicity Studies](#)
- ☐ [Metabolism/Pharmacokinetics](#)
- ☐ [Pharmacology](#)
- ☐ [Environmental Fate & Exposure](#)
- ☐ [Environmental Standards & Regulations](#)
- ☐ [Chemical/Physical Properties](#)
- ☐ [Chemical Safety & Handling](#)
- ☐ [Occupational Exposure Standards](#)
- ☐ [Manufacturing/Use Information](#)
- ☐ [Laboratory Methods](#)
- ☐ [Special References](#)
- ☐ [Synonyms and Identifiers](#)
- ☐ [Administrative Information](#)

ACETONE

CASRN: 67-64-1

For other data, click on the Table of Contents

Human Health Effects:

Toxicity Summary:

Exposure to **acetone** results from both natural and anthropogenic sources. **Acetone** also occurs as a metabolic component in blood, urine and human breath. ... **Acetone** is one of three ketone bodies that occur naturally throughout the body. It can be formed endogenously in the mammalian body from fatty acid oxidation. Fasting, diabetes mellitus and strenuous exercise increase endogenous generation of **acetone**. Under normal conditions, the production of ketone bodies occurs almost entirely within the liver and to a smaller extent in the lung and kidney. ... Products are excreted in the blood and transported to all tissues and organs of the body where they can be used as a source of energy. Two of these ketone bodies, acetoacetate and beta-hydroxybutyrate, are organic acids that can cause metabolic acidosis when produced in large amounts, as in diabetes mellitus. ... Endogenous **acetone** is eliminated from the body either by excretion in urine and exhaled air or by enzymatic metabolism. ... **Acetone** is rapidly absorbed via the respiratory and gastrointestinal tracts of human and laboratory animals, as indicated by the detection of **acetone** in blood within 30 min of inhalation exposure and 20 min of oral administration. ... The nasal cavities of human and laboratory animals appear to have a limited ability to absorb and excrete **acetone** vapor, compared with the remainder of the respiratory tract. **Acetone** is uniformly distributed among non-adipose tissues and does not accumulate in adipose tissue. ... **Acetone** is rapidly cleared from the body by metabolism and excretion. ... Exhalation is the major route of elimination for **acetone** and its terminal metabolite (carbon dioxide), and the fraction of administered **acetone** that is exhaled as unchanged **acetone** is dose-related. Urinary excretion of **acetone** and its metabolites occurs but this route of elimination is minor. ... Exogenously supplied **acetone** enters into many metabolic reactions in tissues throughout the body, but the liver appears to be the site of most extensive metabolism. Carbon from orally administered **acetone** has been detected in cholesterol, amino acids, fatty acids and glycogen in rat tissues, urea in urine and unchanged **acetone** and CO₂ in exhaled breath. Metabolically, **acetone** is degraded to acetate and formate. ... Oral LD₅₀ values in adult rats are in the range of 5800-7138 mg/kg. ... Experimental animal data characterizing the effects of long term oral or inhalation exposure to **acetone** are not available, due probably to its low toxicity and its endogenous characteristics. ... Pretreatment of rodents with **acetone** enhances the hepatotoxic effects of a number of compounds, notably halogenated alkanes. ... **Acetone** is not considered to be genotoxic or mutagenic. ... In a study of pregnant rats and mice exposed to **acetone** vapor during days 6-19 of gestation, slight developmental toxicity was observed. ... Reports of other reproductive effects of **acetone** include observations of testicular effects and changes of sperm quality in rats. ... **Acetone** has been used extensively as a solvent vehicle in skin carcinogenicity studies and is not considered carcinogenic when applied to the skin. **Acetone** is relatively less toxic than many other industrial solvents, however, at high concentrations, **acetone** vapor can cause CNS depression, cardiorespiratory failure and death. Acute exposures of humans to atmospheric concentrations ... have been reported to produce either no gross toxic effects or minor transient effects, such as eye irritation. More severe transient effects (including vomiting and fainting) were reported for workers exposed to **acetone** vapor concentrations ... for about 4 hr. Acute exposures to **acetone** have also been reported to alter performances in neurobehavioral tests in humans. ... Females ... were reported to suffer menstrual irregularities [Environmental Health Criteria 207: Acetone, pp. 1-7 (1998) by the International Programme on Chemical Safety (IPCS) under the joint sponsorship of the United Nations Environment Programme, the International Labour Organisation and the World Health Organization.]**QC REVIEWED**

Evidence for Carcinogenicity:

Contents

Contract all categories

Expand all categories

Select

Clear

- ☐ [FULL RECORD](#)
- ☐ [Human Health Effects](#)
- ☐ [Emergency Medical Treatment](#)
- ☐ [Animal Toxicity Studies](#)
- ☐ [Metabolism/Pharmacokinetics](#)
- ☐ [Pharmacology](#)
- ☐ [Environmental Fate & Exposure](#)
- ☐ [Environmental Standards & Regulations](#)
- ☐ [Chemical/Physical Properties](#)
- ☐ [Chemical Safety & Handling](#)
- ☐ [Occupational Exposure Standards](#)
- ☐ [Manufacturing/Use Information](#)
- ☐ [Laboratory Methods](#)
- ☐ [Special References](#)
- ☐ [Synonyms and Identifiers](#)
- ☐ [Administrative Information](#)

ACETONE

CASRN: 67-64-1

For other data, click on the Table of Contents

Metabolism/Pharmacokinetics:

Metabolism/Metabolites:

Two pathways for the conversion of **acetone** to glucose are proposed, the methylglyoxal & the propanediol pathways. The methylglyoxal pathway is responsible for the conversion to acetol, acetol to methylglyoxal, & subsequent conversion of methylglyoxal to glucose. The propanediol pathway involves the conversion of acetol to L-1,2-propanediol by an as yet unknown process.

L-1,2-propanediol is converted to L-lactaldehyde by alcohol dehydrogenase, & L-lactaldehyde is converted to L-lactic acid by aldehyde dehydrogenase. Expression of these metabolic pathways in rat appears to be dependent on the induction of /**acetone**/ oxygenase & acetol monooxygenase by **acetone**. [Casazza JP et al; J Biol Chem 259 (1): 231-6 (1984)]**PEER REVIEWED**

HEPATIC NAD-DEPENDENT ALCOHOL DEHYDROGENASE ... ENZYME IS CAPABLE OF CATALYZING REVERSE REACTION IN WHICH ... **ACETONE** ... /IS REDUCED TO ALCOHOL/.

[Testa, B. and P. Jenner. Drug Metabolism: Chemical & Biochemical Aspects. New York: Marcel Dekker, Inc., 1976. 310]**PEER REVIEWED**

Acetone may be converted to 1,2-propanediol which enters the glycolytic pathway & possibly the one carbon pool. **Acetone** has been shown to be converted to lactate in mice. The rate-limiting step appears to be the conversion of **acetone** to a hydroxylated intermediate. Rats & mice exposed to 30 mg/l of **acetone**, & rabbits & guinea pigs exposed to 72 mg/l for 2 hr, had increased levels of **acetone**, acetoacetic acid, & beta-hydroxybutyric acid in the blood & urine immediately after exposure & 24 hr later.


[Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982. 4726]**PEER REVIEWED**

Acute admin of **acetone** to rats resulted in measureable levels of isopropanol in blood. Metabolism of

Links to Related Records in Other Databases ...

[IRIS Record](#)[CCRIS Record](#)[GENETOX Record](#)[TOXLINE SPECIAL Records](#)[TOXLINE CORE Records](#)

Contents

Contract all categories Expand all categories 

Select

Clear

- ☐  [FULL RECORD](#)
- ☐  [Substance Identification](#)
 - ☐  [Substance Name](#)
 - ☐  [CAS Registry Number](#)
 - ☐  [Data Type](#)
- ☐  [Studies Data](#)
 - ☐  [Mutagenicity Studies](#)
- ☐  [Administrative Information](#)
 - ☐  [CCRI5 Record Number](#)
 - ☐  [Last Revision Date](#)
 - ☐  [Update History](#)

ACETONE

CASRN: 67-64-1

*For other data, click on the Table of Contents***Substance Identification:**

Substance Name: ACETONE

CAS Registry Number: **67-64-1**

Data Type:

Mutagenicity


Studies Data:**Mutagenicity Studies:**

Test System:	AMES SALMONELLA TYPHIMURJUM
Strain Indicator:	TA100
Metabolic Activation:	NONE
Method:	PREDNCUBATION
Dose:	100-10000 UG/PLATE (TEST MATERIAL SOLVENT: DISTILLED WATER)
Results:	NEGATIVE
Reference:	

[ZEIGER, E, ANDERSON, B, HAMORTH, S, LAWLOR, T AND MORTELMANS, K; SALMONELLA MUTAGENICITY TESTS. V. RESULTS FROM THE TESTING OF 311 CHEMICALS; ENVIRON. MOL. MUTAGEN. 19(SUPPL.21):2-141, 1992]


Test System:	AMES SALMONELLA TYPHIMURJUM
Strain Indicator:	TA100
Metabolic Activation:	HAMSTER, LIVER, S-9, AROCLOR 1254 (10 OR 30%)
Method:	PREDNCUBATION

LIMITS



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Hazardous Substances Data Bank

[Tox. & Env. Health](#) [TOXNET](#) [HSDB](#) [Limits](#)

Databases

Search HSDB

Hazardous Substances Data Bank

IRIS

GENE-TOX

CCRIS

Multi-Databases

TOXLINE

DART/ETIC

TRI

ChemIDplus

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[Tox Weblinks](#)
[MEDLINEplus](#)
[Tox Env. Health subset](#)
[PubMed](#)
[NLM Gateway](#)
[Locatorplus](#)

Support Pages

[Help](#)
[Fact Sheet](#)
[Sample Record](#)
[HSDB Scientific Review Panel](#)

Add chemical synonyms and CAS numbers to search: ☒ Yes ☐ No

Search: ☐ exact words ☒ singular & plural forms ☐ word variants
Search records with: ☒ the phrase ☐ all words ☐ any words

Search in fields:
(If no box is checked, all fields will be searched.)

☐ ☐ Substance Identification
☒ ☐ Human Health Effects
☐ ☐ Emergency Medical Treatment
☐ ☐ Animal Toxicity Studies
☐ ☐ Metabolism/Pharmacokinetics
☐ ☐ Pharmacology
☐ ☐ Environmental Fate & Exposure
☐ ☐ Environmental Standards & Regulations
☐ ☐ Chemical/Physical Properties
☐ ☐ Chemical Safety & Handling
☐ ☐ Occupational Exposure Standards
☐ ☐ Manufacturing/Use Information
☐ ☐ Laboratory Methods
☐ ☐ Special References
☐ ☐ Synonyms and Identifiers

Search History

- To review search strategies
- To combine search statements (within databases)
- Query Box provided to enter subsequent searches directly on Search History Page
- Use # to combine search statements (e.g. #1 AND #2)

Search *HSDB* for **#1 AND #2**

- Search History will be lost after one hour of inactivity.
- To combine searches use # before search number: e.g. #2 AND #6
- Searches may not be combined across databases.

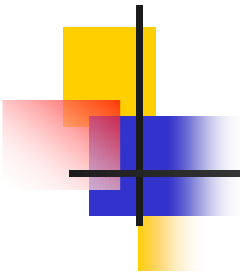
Search	Database	Query	Time	Result
# 2	hsdb	[use] [mfs] [mmfg] [omni] [form] [imp] [cpat] [prod] [imgt] "latex paint" [expt]	10:12:24	19
# 1	hsdb	[toos] [care] [htox] [htox] [serv] [warn] [meds] [popl] [rtex] [body] [avdi] "lymphatic leukemia" [minf]	10:12:03	5

Clear History



Boolean Searching, Field Qualification, Search Techniques

- Upper Case Boolean Operators (AND, OR, NOT)
- Fields in brackets and post-qualified (e.g. benzene [na])
- Nested parenthesis permitted
- Phrase searching with quotation marks (e.g. “coronary artery bypass”)
- Asterisk (*) for truncation (e.g. carcinogen*)



Part III

TOXLINE and Related Files



TOXLINE

TOXicology Literature onLine

- Covers pharmacological, biochemical, physiological, environmental, and toxicological effects of chemicals/other agents on living systems
- Citations, Abstracts, Keywords and/or MeSH (Medical Subject Headings)
- CAS Registry Numbers
- From 1965 to date (and earlier)
- Drawn from Secondary Sources, varying unit record formats
- Components – TOXLINE Core (on PubMed, accessible via TOXNET) and TOXLINE Special (on TOXNET)
- Over 3 million toxicology related records combined



TOXLINE Core (on PubMed)

- Toxicology Subset limit of MEDLINE on PubMed
- Similar to TOXLINE's former TOXBIB subfile
- Drawn from standard biomedical journal literature
- Accessible directly on PubMed or from the TOXLINE search screen on TOXNET
- Some features of PubMed:
 - MeSH Searching
 - Limit by field, publication type, age, gender, language, human or animal, etc.
 - Cubby – to store and update searches
 - Related articles
 - LinkOut
 - Interlibrary Loan (Loansome Doc)



TOXLINE Special (on TOXNET)

- Technical Reports and Research projects
 - Federal Research in Progress (FEDRIP)
 - Toxicology Document and Data Depository (NTIS)
 - Toxicology Research Projects (CRISP)
 - Toxic Substances Control Act Test Submissions (TSCATS)

- Special Journal and Other Research Literature
 - Developmental and Reproductive Toxicology (DART)
 - International Labour Office (CIS)
 - Swedish National Chemicals Inspectorate (RISKLINE)



TOXLINE Special (continued)

- Archival Collections (No Longer Being Updated)
 - Aneuploidy (ANEUPL)
 - Environmental Mutagen Information Center file (EMIC)
 - Environmental Teratology Information Center file (ETIC)
 - Epidemiology Information System (EPIDEM)
 - Hazardous Materials Technical Center (HMTC)
 - International Pharmaceutical Abstracts (IPA)
 - NIOSHTIC (NIOSH)
 - Pesticides Abstracts (PESTAB)
 - Poisonous Plants Bibliography (PPIB)
 - Toxicological Aspects of Environmental Health (BIOSIS)



TOXLINE Special (continued)

- Some Features of TOXLINE Special
 - Relevancy Ranking
 - Toggle between TOXLINE Special and TOXLINE Core
 - Automatic Mapping to MeSH terms
 - Link to TOXLINE Special from *ChemIDplus*

Note: Search algorithms and display formats of TOXLINE Special and TOXLINE Core vary.



Another Toxicology Literature File

Developmental and Reproductive Toxicology (DART/ETIC)

100,000 Records

- Covers Developmental and Reproductive Toxicology (including Teratology)
- Components – DART Core (on PubMed) and DART Special (on TOXNET)



Search Page - Toxicology Literature Files

- One Box Search for:
 - Chemicals – enter chemical names or CAS Registry numbers.
Let system add synonyms (default) or use exact terms entered.
 - Other Terms
- Field Limits – All, Title, Author (e.g. Smith H)
- Publication Year Limits – Any, 1998-, 1990, 1980-
- Browse Index for:
 - All Words
 - Authors
 - MeSH Headings/Keywords
 - CAS Registry Numbers
- Automatic Term Mapping to MeSH & UMLS
 - e.g. passive smoking --- tobacco smoke pollution
- Limits
 - For more precise searching – to search within all fields, title only, author only, by specific year of publication, subfile, language, etc.



Search Results Page - Toxicology Literature Files

- Displays title, author, source, subfile of retrieved records
- Relevancy Ranked Display
- Select Record(s) of Interest
- View Details of Search Strategy
- Modify Search – Returns you to Search Page with query intact
- Begin a new Basic Search – Returns you to Search Page with blank query box
- Or Search can be modified or begun anew directly on Results Page
- Sort Results – By year of publication, title, author, entry month, relevance, in ascending or descending order
- Save Checked Items, Display Checked Items
- View Search History and combine search statements
- Download – Brief, Full, Abstract, Tagged
- Browse Index
- Return to TOXNET Home



Selected Record Page - Toxicology Literature Files

- Displays full bibliographic record – Title, Author, Source, Abstract, keywords, etc.
- **Search Terms highlighted in Red**
- **Hot Linked Items (e.g. authors, keywords, CAS registry numbers) highlighted and underlined, in Blue**
- Related Records
- Return to Search Results page
- Download – Brief, Full, Abstract, Tagged
- Modify Search – Returns you to Search Screen with query intact
- Begin a new Basic Search – Returns you to search Screen with blank query box
- Or Search can be modified or begun anew directly on Results Page
- View Details of Search Strategy
- View Search History and combine search statements
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Toxicology Bibliographic Information

[Tox. & Env. Health](#) [TOXNET](#) [TOXLINE](#)

Databases

HSDB	i
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CCRIS	i
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DART/ETIC	i
TRI	i
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Search TOXLINE

brain cancer pesticides

Search

Clear

For chemicals, add synonyms
and CAS numbers to search:

☒ Yes ☐ No

Search in

- ☒ TOXLINE Special
☐ TOXLINE Core on PubMed
☐ Both

Limits

Browse the Index

Other NLM Resources

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TOXLINE Special Search Results

► [Tox. & Env. Health](#) ► [TOXNET](#) ► [TOXLINE Special](#)

Save
Checked Items

Sort

Details

History

Download

Modify Search

Basic Search

Browse Index

TOXNET Home

brain cancer pesticides

Search

Clear

Limits

For chemicals, add synonyms and CAS numbers to search: ☒ Yes ☐ No

Items 1 through 20 of 60

Pages: [1](#) [2](#) [3](#) ►

References are sorted in [relevancy ranked](#) order.

Click on Sort to change the order of the retrieved References.

Select Record

Reference

- 1 ☐ [Pesticide prioritization for a brain cancer case-control study.](#)
Sanderson WT; Talaska G; Zaebst D; Davis-King K; Calvert G
Environ Res 1997;74(2):133-44 [DART]
- 2 ☐ [Pesticide Prioritization for a Brain Cancer Case-Control Study](#)
Sanderson WT; Talaska G; Zaebst D; Davis-King K; Calvert G
Environmental Research, Vol. 74, No. 2, pages 133-144, 28 references, 1997 [NIOSH]
- 3 ☐ [Pesticide prioritization for a brain cancer case-control study.](#)
SANDERSON WT; TALASKA G; ZAEBST D; DAVIS-KING K;
CALVERT G
ENVIRONMENTAL RESEARCH; 74 (2). 1997. 133-144. [BIOSIS]
- 4 ☐ [Occupational Risk Factors for Brain Tumors among Women in Shanghai, China](#)
Heineman EF; Gao Y-T; Dosemeci M; McLaughlin JK
Journal of Occupational and Environmental Medicine, Vol. 37, No. 3, pages 288-293, 22 references, 1995 [NIOSH]
- 5 ☐ [Brain cancer mortality among French farmers: The vineyard pesticide hypothesis.](#)
VIEL J-F; CHALLIER B; PITARD A; POBEL D
ARCHIVES OF ENVIRONMENTAL HEALTH; 53 (1). 1998. 65-70. [BIOSIS]
- 6 ☐ [Family pesticide use and childhood brain cancer.](#)
DAVIS JR; BROWNSON RC; GARCIA R; BENTZ BJ; TURNER A
ARCH ENVIRON CONTAM TOXICOL; 24 (1). 1993. 87-92. [BIOSIS]
- 7 ☐ [What causes childhood brain tumors? Limited knowledge, many clues.](#)
Bunin G



Related
Records

Search Results

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Browse Index

Modify Search

Details

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brain cancer pesticides

Search

Clear

Limits

For chemicals, add synonyms and CAS numbers to search: ☒ Yes ☐ No

Item 1 of 60
[PubMed Record](#)

Pesticide prioritization for a brain cancer case-control study.

Authors:

[Sanderson WT](#)
[Telaska G](#)
[Zachat D](#)
[Davis-King K](#)
[Calvert G](#)

Author Address: National Institute for Occupational Safety and Health, Cincinnati, Ohio 45226, USA. wts1@cdc.gov

Source: Environ Res 1997;74(2):133-44

Abstract:

The incidence of **brain cancer** is rising in the United States while the causes remain largely unknown. Epidemiologic studies indicate that individuals working in agriculture have an increased risk of **brain cancer**. The National Institute for Occupational Safety and Health is conducting a case-control study of incident **brain cancer** cases in Iowa, Michigan, Minnesota, and Wisconsin to evaluate the risk associated with several environmental exposures, in particular agricultural **pesticides**. Hundreds of different **pesticides** are used in agriculture and it is not feasible to evaluate the association between **brain cancer** and exposure to each of these chemicals; therefore, a strategy was developed to identify which **pesticides** would be targeted in the study. First lists of **pesticides** were created, documenting usage in each of the four states and the United States as a whole, by using data from reports prepared by the U.S. Department of Agriculture and Departments of Agriculture and land grant colleges within the four states. Then the following factors were considered in prioritizing **pesticides** for evaluation in the study: total volume of use prior to 1985, ranking of use in the four states and the United States as a whole by **pesticide** category, and toxicological evidence of carcinogenic, teratogenic, or mutagenic effects. **Pesticide** usage prior to 1985 was determined to allow for a minimum 10-year latency for the incident **brain cancer** cases diagnosed in 1995 or later. The selected **pesticides** include 56 herbicides, 49 insecticides, 12 fungicides, and 17 fumigants, accounting for over 99% of the total pounds of herbicides and insecticides and over 98% of the total pounds of fungicides and fumigants applied pre-1985. Prompt lists of the **pesticides** are sent to study participants a few days before the study questionnaire is administered to allow them time to recall past use of **pesticides**; the lists include the common chemical names, trade names, the crops that the **pesticides** are most commonly used on, and the years that the **pesticides** have been marketed. The methods used to select this subset of 134 **pesticides** document historical usage and may be useful in prioritizing **pesticides** for other research studies.

Medical Subject Headings (MeSH):

[Brain Neoplasms/CHEMICALLY INDUCED](#)

[Brain Neoplasms/*EPIDEMIOLOGY](#)

[Case-Control Studies](#)

[Environmental Exposure](#)

[Human](#)

[Incidence](#)

[Pesticides/*POISONING](#)

[Support, U.S. Gov't, P.H.S.](#)

[United States/EPIDEMIOLOGY](#)

Substance (CAS Registry Number):

[Pesticides](#) (NO CAS RN)

Language: English

International Standard Serial Number: 0013-9351

Publication Types:

JOURNAL ARTICLE

Entry Month: January, 1998

Journal Title Code: EI2

Title Abbreviation: Environ Res

Year of Publication: 1997

Secondary Source ID: DART/MED/[97480528](#)

Last Revision Date: December 30, 1997

Search for

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Limits: Toxicology

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☐ 1: [Markovsky M](#)

Thiran inhibits angiogenesis and slows the development of experimental tumours in mice.

Br J Cancer. 2002 Mar 4;86(5):779-87.

PMID: 11875743 [PubMed - indexed for MEDLINE]

[Related Articles](#)

☐ 2: [Slaughter MR](#), [Thakkar H](#), [O'Brien PJ](#)

Effect of diquat on the antioxidant system and cell growth in human neuroblastoma cells.

Toxicol Appl Pharmacol. 2002 Jan 15;178(2):63-70.

PMID: 11814326 [PubMed - indexed for MEDLINE]

[Related Articles](#)

☐ 3: [Maeda K](#), [Gotoh H](#), [Chikui E](#), [Furusawa T](#)

Intratumoral hemorrhage from a posterior fossa tumor after cardiac valve surgery--case report.

Neurol Med Chir (Tokyo). 2001 Nov;41(11):548-50.

PMID: 11758708 [PubMed - indexed for MEDLINE]

[Related Articles](#)

☐ 4: [Mills PK](#), [Zahn SH](#)

Organophosphate pesticide residues in urine of farmworkers and their children in Fresno County, California.

Am J Ind Med. 2001 Nov;40(5):571-7.

PMID: 11675626 [PubMed - indexed for MEDLINE]

[Related Articles](#)

☐ 5: [Gurney JG](#), [Smith MA](#), [Olshan AF](#), [Hecht SS](#), [Kasam CM](#)


Clues to the etiology of childhood brain cancer: N-nitroso compounds, polyomaviruses, and other factors of interest.

Cancer Invest. 2001;19(6):630-40. Review. No abstract available.

PMID: 11486706 [PubMed - indexed for MEDLINE]



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Add chemical synonyms and CAS numbers to search:
☒ Yes ☐ No

Search in:
☐ TOXLINE Special
☐ TOXLINE Core on PubMed
☒ Both

Search fields:
☐ All fields
☒ Titles
☐ Authors (e.g., Smith H)

Search: ☐ exact words ☒ singular & plural forms ☐ word variants
Search records with: ☐ the phrase ☒ all words ☐ any words

Maximum records returned

Year of Publication:
 through

Only search documents added in the last months.

TOXLINE Components

Language

All

ANEUPL

BIOSIS

CIS

CRISP

DART

All

English

Afrikaans

Arabic

Armenian

Azerbaijani

To select more than one component, click while holding the CTRL (PC) or CMD (Mac) key.

TOXLINE Special
Search Results

beryllium workers

For chemicals, add synonyms and CAS numbers to search

Items 1 through 19 of 19

References are sorted in [relevancy ranked](#) order.
Click on **Sort** to change the order of the retrieved References

Select
Record

Reference

- 1 ☐ [CHRONIC BERYLLIUM DISEASE AMONG BER](#)
ROSSMAN M
Crisp Data Base National Institutes of Health [CR
- 2 ☐ [VALUE OF THE LYMPHOCYTE BLAST TRANSF](#)
[BERYLLIUM HYPER SENSITIVITY IN BERYLLI](#)
[EXPERIENCE](#)
VANORDSTRAND HS
GEE, J. B. L., W. K. C. MORGAN AND S. M. BRO
LUNG DISEASE; INTERNATIONAL CONFERENCE
27, 1982. XXXI+264P. RAVEN PRESS: NEW YOR
89004-900-9; 0 (0). 1984. P220-221. [HEEP]
- 3 ☐ [CHRONIC BERYLLIUM DISEASE AMONG BER](#)
ROSSMAN M
Crisp Data Base National Institutes of Health [CR
- 4 ☐ [Beryllium exposure and pulmonary function: A cross sectional study of](#)
[beryllium workers](#)
Kriebel D ; Sprince NL ; Eisen EA ; Greaves IA ; Feldman HA ; Greene RE
British Journal of Industrial Medicine Mar. 1988, Vol.45, No.3, p.167-173. 13 ref.
[CIS]
- 5 ☐ [Reversible beryllium sensitization in a prospective study of beryllium](#)
[workers.](#)
ROM WN ; LOCKEY JE ; BANG KM ; DEWITT C ; JOHNS R E JR
ARCH ENVIRON HEALTH; 38 (5). 1983. 302-307. [HEEP]
- 6 ☐ [BERYLLIUM EXPOSURE AND PULMONARY FUNCTION A CROSS SECTIONAL](#)
[STUDY OF BERYLLIUM WORKERS](#)
KRIEBEL D ; SPRINCE NL ; EISEN EA ; GREAVES IA ; FELDMAN HA ; GREENE RE
BR J IND MED; 45 (3). 1988. 167-173. [BIOSIS]
- 7 ☐ [Reversible beryllium sensitization in a prospective study of beryllium](#)
[workers](#)
Rom WN ; Bang KM ; Dewitt C ; Johns RE ; Locky JE



for [beryllium\[TI\] workers\[TI\] AND 1900:2002\[dp\] AND](#) Go Clear

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Display Summary Sort Save Text Clip Add Order

Show: 20 Items 1-20 of 27 Page 1 of 2 Select page: 1 2

☐ 1: [Deubner DC, Lockey JL, Kotin P, Powers MB, Miller F, Rogers AE, Trichopoulos D.](#) [Related Articles](#)

Re: Lung cancer case-control study of beryllium workers. Sanderson WT, Ward EM, Steenland K, Petersen MR. Am J Ind Med. 2001. 39:133-144.
Am J Ind Med. 2001 Sep;40(3):284-8. No abstract available.
PMID: 11598976 [PubMed - indexed for MEDLINE]

☐ 2: [Henneberger PK, Cumro D, Deubner DD, Kent MS, McCawley M, Kreiss K.](#) [Related Articles](#)

Beryllium sensitization and disease among long-term and short-term workers in a beryllium ceramics plant.
Int Arch Occup Environ Health. 2001 Apr;74(3):167-76.
PMID: 11355290 [PubMed - indexed for MEDLINE]

Save
Checked Items

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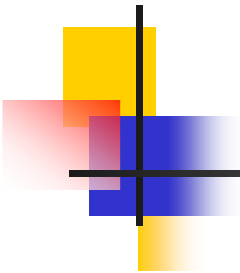
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TOXNET Home



Part IV

TRI and other Specialty Files



Toxics Release Inventory (TRI)

U.S. Environmental Protection Agency (EPA)

TRI 95-00 – 482,531 Records

- Facility Identification (Facility Name, Address, Phone, etc.)
- Substance Identification (Chemical Name, CAS RN, Uses, etc.)
- Environmental Release of Chemical (in Air, Water, Land, Underground Injection)
- Waste Treatment
- Off-Site Waste Treatment
- Source Reduction and Recycling (Quantity Released, Energy Recovery, Quantity Recycled, Quantity Treated)



TRI Background

- Right-to-Know Movement – Workplace, Community
- OSHA Hazard Communication Standard – 1983
- SUPERFUND = CERCLA (1980)
- Bhopal (1984) and smaller scale chemical disasters
- SARA (Superfund Amendments and Reauthorization Act) (1986)
 - Title 3 = Emergency Planning and Community Right-to-Know Act
 - Section 313 = Toxic Release Reporting
- Pollution Prevention Act of 1990



Search Page - TRI

- Several search query boxes – fill in any combination.
- Chemical names or CAS Registry numbers. Let system add synonyms (default) or use exact terms entered.
- Select Year(s) – 1995-2000
- Facility Name(s)
- Facility Location (state, city/state, county/state, zip)
- Ranging
 - Greater than _____ pounds
 - Total Release, Air, Water, Land, Underground Injection
 - Or “No Release Selected”
- Browse Index for:
 - All Words
 - Chemical Name
 - CAS Registry Number
 - Facility Name
 - Facility City



Search Results Page - TRI

- Displays facility name, chemical, city/state of retrieved records.
- Unsorted order
- Select Record(s) of Interest
- Calculate Releases – Tabular Display of Total Environmental Releases and Off-Site Waste Transfers for all retrieved records.
- View Details of Search Strategy
- Modify Search – Returns you to Search Page with query intact
- Begin a new Basic Search – Returns you to Search Page with blank query box (note: search screen can't be modified directly from this page)
- Sort Results – By substance name, facility name, city, or state. Ascending or Descending.
- Save Checked Items, Display Checked Items
- View Search History and combine search statements
- Download – Brief or Full Format
- Browse Index
- Return to TOXNET Home



Selected Record Page - TRI

- Full record displayed
- Choose fields for display from Contents (expand, contract categories)
- Navigate – Next Item, Previous Item
- View Details of Search Strategy
- Modify Search – Returns you to Search Screen with query intact
- Begin a New Search – Returns you to Search Screen with blank query box
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- Download – In Full Format
- Return to TOXNET Home
- Link to records for the same chemical in Other Files



Toxics Release Inventory

[Tox. & Env. Health](#) [TOXNET](#) [TRI](#)

Databases

HSDB



IRIS



GENE-TOX



CCRIS



Multi-Databases



TOXLINE



DART/ETIC



Toxics Release
Inventory



ChemIDplus



TOXNET Home

Search TRI

Other NLM Resources

Chemical Name or CAS Registry Number

methyl ethyl ketone

Search

Clear

Add synonyms and CAS numbers to search:

☒ Yes ☐ No

☐ TRI2000 ☒ TRI99 ☐ TRI98

☐ TRI97 ☐ TRI96 ☐ TRI95

Facility Names

(Separate multiple entries with commas)

Facility Location

marshfield/mo

☐ State ☒ City/State

☐ County/State ☐ Zip

Greater Than for

Search

Browse the Index

[DIRLINE](#)

[Haz-Map](#)

[AltBib](#)

[Tox Weblinks](#)

[MEDLINEplus](#)

[Tox/Env. Health subset](#)

[PubMed](#)

[NLM Gateway](#)

[Locatorplus](#)

Support Pages

[Help](#)

[Fact Sheet](#)

[Sample Record](#)



TRI99 Search Results

[Tox. & Env. Health](#) [TOXNET](#) [TRI99](#)

Calculate
Release!

Save
Checked Items

Sort

Details

History

Download

Modify Search

New Search

Browse Index

TOXNET Home

Please click on **Modify Search** button to modify TRI search strategy.

Items **1** through **2** of **2**

*Facility/Substance Names are **unsorted**.*

Select Record	Facility/Substance Name
1 <input type="checkbox"/>	WILCORP INDS. INC. METHYL ETHYL KETONE MARSHFIELD, MO
2 <input type="checkbox"/>	YORK CASKET-MISSOURI METHYL ETHYL KETONE MARSHFIELD, MO

Contents

[Contract all categories](#)[Expand all categories](#)[Select](#)[Clear](#)

- ☐ [FULL RECORD](#)
- ☐ [Facility Identification](#)
- ☐ [Substance Identification](#)
- ☐ [Environmental Release of Chemical](#)
- ☐ [Waste Treatment](#)
- ☐ [Off-Site Waste Transfer](#)
- ☐ [Source Reduction and Recycling](#)
- ☐ [Administrative Information](#)

TRI99

METHYL ETHYL KETONE

YORK CASKET-MISSOURI

MARSHFIELD, MO

For other data, click on the Table of Contents

Environmental Release of Chemical:**Non-Point Air Emissions Estimates:**

Non-Point Air Release: 1,900 lbs./rep yr. 1999

Basis of Estimate: (C) Mass Balance Calculations

Point Air Emissions Estimates:

Point Air Release: 17,000 lbs./rep yr. 1999

Basis of Estimate: (C) Mass Balance Calculations

Total Air Release: 18,900 lbs./rep yr. 1999

Water Discharge Estimates:

Receiving Stream: NA

Water Release: NA

Basis of Estimate: 0%

Total Water Release: 0 lbs./rep yr. 1999

Underground Injection Total: 0 lbs./rep yr. 1999

Land Release Estimates:

Disposal Method: (D03) Land Treatment/Application/Farming

Land Release: NA



Search as    

[Haz-Map Search](#)

[More Searches](#)

[Haz-Map Help](#)

[Glossary](#)

[References](#)

Browse Haz-Map

- [Hazardous Agents](#)

1. [By Types of Agents](#)
2. [By Adverse Effects](#)
3. [Alphabetically](#)

- [Occupational Diseases](#)

1. [By Types of Diseases](#)
2. [By **Jobs** and **Symptoms**](#)
3. [Alphabetically](#)

- [High Risk Jobs](#)

1. [By Types of Jobs](#)
2. [Alphabetically](#)

[Haz-Map](#): Information on Hazardous Chemicals and Occupational Diseases
by
[Jay A. Brown, MD., M.P.H.](#)

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Last updated: May 8, 2002



Search as    

[Haz-Map Search](#)

[More Searches](#)

[Haz-Map Help](#)

[Glossary](#)

[References](#)

[Browse Haz-Map by Jobs](#)

[Search TOXNET](#)

Information about this job:

Carpenters

• **High risk job tasks associated with this job:**

- [Apply arsenic preservatives to wood](#)
- [Contaminate skin or inhale spray while using pentachlorophenol](#)
- [Handle agents that cause allergic contact dermatitis or contact urticaria](#)
- [Installed insulation before 1975](#)
- [Machine allergenic wood and inhale dust](#)
- [Remove insulation installed before 1975](#)
- [Saw or sand arsenic-treated wood](#)
- [Saw or sand creosote-treated wood](#)
- [Use epoxy, isocyanate, or formaldehyde-resin adhesives, finishes, or sealants](#)
- [Use n-hexane as a solvent in glues, coatings, and degreasers](#)
- [Work with glue solvents](#)

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Last updated: May 8, 2002



Search

as



Agent



Disease



Job



Text Search

[Haz-Map Search](#)

[More Searches](#)

[Haz-Map Help](#)

[Glossary](#)

[References](#)

[Browse Haz-Map](#)

[Search TOXNET](#)

Agent Name	n-Hexane
Alternative Name	Hexane
<u>CAS Number</u>	110-54-3
Formula	C6-H14
Major Category	Solvents
Synonyms	Hexyl hydride, normal-Hexane
Category	Alkanes (Paraffins)
Description	Colorless liquid with a gasoline-like odor;
Sources/Uses	Used as a solvent, especially in the adhesive and shoe industries; abused by glue sniffers for its euphoric effects; [LaDou, p. 371] Used in shoe and furniture manufacture to dissolve glue; also used in adhesive tape manufacturing; [Sullivan, p. 1124]
Comments	n-Hexane is in the list of "Some volatile substances which may be abused by inhalation" published on the web site of the U.N. International Drug Control Programme, indicating its potential to cause narcosis in workers. In addition to CNS solvent syndrome, n-Hexane can cause motor neuropathy.

Exposure Assessment	
<u>BEI</u>	2,5-Hexanedione in urine = 5 mg/g creatinine; end of shift; screen for n-hexane in end-expired air; ACGIH Notice of Intended Change (2001): 2,5-Hexanedione (free) in urine = 4 mg/L end of shift near end of workweek;
<u>Skin Designation (ACGIH)</u>	Yes
<u>TLV (ACGIH)</u>	50 ppm
<u>PEL (OSHA)</u>	500 ppm
<u>IDLH (NIOSH)</u>	1100 ppm
<u>Excerpts from Documentation for IDLHs</u>	It has been reported that a 10-minute exposure to 5,000 ppm caused dizziness and a sensation of giddiness.
<u>Vapor Pressure</u>	124 mm Hg
<u>Odor Threshold Low</u>	65 ppm
<u>Odor Threshold High</u>	248 ppm
<u>Explanatory Notes</u>	IDLH = 10% of LEL (lower explosive limit); Odor threshold from AIHA;
<u>MAK</u>	50 ppm
<u>Half Life</u>	Urine (2,5-hexanedione): 15 hours; blood: 2-3 hours; fat: 64 hours; [TDR, p. 1480]
<u>Reference Link</u>	ATSDR ToxFAQs - n-Hexane
<u>Flammability (NFPA)</u>	3: may ignite at ambient temperature
Adverse Effects	
<u>Neurotoxin</u>	Motor Neuropathy

Household Products Database

Home

Products

Ingredients

Health

Welcome

About

Contact Us

Web Resources

[Cornell University
PDC MSDS Search](#)
[Vermont SIRI MSDS
Archive](#)

NLM Resources

[TOXNET](#)
[MEDLINEplus](#)
[PubMed](#)

Health & Safety Information on Household Products

What's under your kitchen sink, in your garage, in your bathroom, and on the shelves in your laundry room? Do these household products pose a potential health risk to you and your family?

Find out what's in these products and what are the potential health effects, and other safety and handling information.

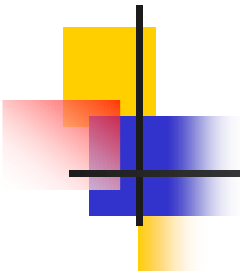
[Continue...](#)



PROTOTYPE –

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Last updated: November 5, 2001



Part V

Non-NLM Resources



Professional Associations

- Society of Toxicology – <http://www.toxicology.org/>
- Society of Environmental Toxicology and Chemistry – <http://www.setac.org>
- American Academy of Clinical Toxicology – <http://www.clintox.org>
- American Association of Poison Control Centers – <http://www.aapcc.org>
- Society of Risk Analysis – <http://www.sra.org>
- Other groups in environmental health, occupational health, industrial hygiene, health physics etc.



U.S. Government Resources

- Agency for Toxic Substances and Disease Registry (ATSDR) – <http://www.atsdr.cdc.gov>
- Environmental Protection Agency (EPA) – <http://www.epa.gov>
- Food and Drug Administration – <http://www.fda.gov>
 - National Center for Toxicological Research – <http://www.fda.gov/nctr>
- National Institute for Occupational Safety and Health – <http://www.cdc.gov/niosh>



U.S. Government Resources (continued)

- National Institute of Environmental Health Sciences – <http://www.niehs.nih.gov>
- National Toxicology Program – <http://ntp-server.niehs.nih.gov>
- U.S. Chemical Safety and Hazard Investigation Board – <http://www.chemsafety.gov>

Some State Government Sites

- New Jersey Department of Health and Senior Services – Division of Epidemiology, Environmental and Occupational Health – <http://www.state.nj.us/health/eoh>
- California – Office of Environmental Health Hazard Assessment – <http://www.oehha.ca.gov>



Some Chemical Databases

- Chemfinder – <http://www.chemfinder.com>
- International Toxicity Estimates for Risk (ITER) (from TERA) (featuring comparative risk values) – <http://www.tera.org/iter>
- Scorecard (from Environmental Defense) – <http://www.scorecard.org>
- Environmental Fate Databases & more (from Syracuse Research Corporation) – <http://esc.syrres.com>
- EXTtoxNET (pesticide information) – <http://ace.orst.edu/info/extoxnet>



Some Chemical Databases (continued)

- PAN (Pesticide Action Network) Pesticides Database – <http://www.pesticideinfo.org>
- Where to Find Material Safety Data Sheets on the Internet – <http://www.ilpi.com/msds>
- RxList, the Internet Drug Index – <http://www.rxlist.com>
- International Programme for Chemical Safety (IPCS) INCHEM – <http://www.inchem.org/search.html>



Other Web Sites

- UNEP (United Nations Environment Programme) Chemicals – <http://www.chem.unep.ch>
- Intergovernmental Forum on Chemical Safety - <http://www.who.int/ifcs/>
- Inter-Organization Programme for the Sound Management of Chemicals - <http://www.who.int/iomc/>
- National Council for Science and the Environment – <http://www.cnie.org>
- Society of Environmental Journalists – <http://www.sej.org>
- TEHIP/NLM Web Links – <http://sis.nlm.nih.gov/Tox/ToxWebLinks.html>



Some Commercial (\$) Databases

- ARIEL Insight – Ariel Research – <http://www.arielresearch.com>
- BIOSIS Previews – BIOSIS – <http://www.biosis.org>
- Chemical Abstracts & CAS Registry – Chemical Abstracts Service – <http://www.cas.org> (also <http://stnweb.cas.org>)
- CCINFOweb (CHEMINDEX & IPCS/INCHEM are free) – CCOHS – <http://www.ccohs.ca>
- CISILO Database (on occupational health) (from the International Labour Office) (free as a TOXLINE subfile) – <http://www.ilo.org>



Some Commercial (\$) Databases (continued)

- EMBASE – Elsevier Science – <http://www.embase.com>
- Environment Abstracts – Congressional Information Service – <http://www.cispubs.com>
- MICROMEDEX Databases – MICROMEDEX – <http://www.micromedex.com>
- Toxicology Abstracts – Cambridge Scientific Abstracts – <http://www.csa.com>
- Web of Science – ISI – <http://www.isinet.com/isi/products/citation/wos/>



Some Web Search Engines and Tools

- AltaVista – <http://www.altavista.com>
- Google – <http://www.google.com>
- Hotbot – <http://www.hotbot.com>
- Yahoo – <http://www.yahoo.com>
- Meta Search Engines
 - Go2Net – <http://www.go2net.com>
 - Dogpile – <http://www.dogpile.com>
 - Ask Jeeves – <http://www.askjeeves.com>
- Searchenginewatch – <http://www.searchenginewatch.com>
- Mailing Lists & Newsgroups – <http://www.liszt.com>

TOXNET Exercises

[Note: There is typically more than one “right” answer to each of the following questions. Answers, where they are provided, are merely representative, not definitive. Explore.]

TOXICOLOGY DATA FILES

1. What is the CAS registry number and octanol/water partition coefficient of 2,6-dinitrotoluene and what is this chemical used for? [HSDB]

In HSDB, search for **2,6-dinitrotoluene** and click on the 2,6-dinitrotoluene record on the Search Results Page. In the Table of Contents, expand **Chemical/Physical Properties** and click on **Octanol/Water Partition Coefficient**. Expand **Manufacturing/Use Information** and click on **Major Uses**.

2. Has 2,6-dinitrotoluene been shown to be mutagenic in the Ames salmonella test? [HSDB]

MODIFY above search to **2,6-dinitrotoluene ames**.

3. What is the oral LD50 of caffeine in male rabbits? Also, click on **DETAILS** to view the search strategy. [HSDB]

Search for **oral ld50 caffeine male rabbits** and click on **caffeine** record.

4. Has caffeine been studied as a tumor promoter? Does it cause mutations? [CCRIS, GENE-TOX]

From HSDB caffeine record (above), click on **Other Files**. Select CCRIS. Expand Studies in Table of Contents and check the boxes for **Tumor Promotion Studies** and **Mutagenicity Studies**. Return to HSDB. Click on **Other Files** again and select GENE-TOX. **Select Mutagenicity Studies**.

5. Which of the toxicology data files contain information on ammonia? What is the Inhalation Reference Concentration (RfC) of ammonia? (Note: the RfC is a non-carcinogenic risk assessment parameter) Also, view the DOWNLOAD options available. [Multi-Data Base and IRIS]

Select the **Multi-Database** option on the TOXNET main page. Search for **ammonia**. Click on the IRIS ammonia record. Expand **Chronic Health Hazard Assessment for Noncarcinogenic Effects** in Table of Contents. Click on **Reference Concentration for Chronic Inhalation Exposure (RfC)**.

TOXNET Exercises (continued)

6. What are some chemicals used in leather tanning and what are their human health effects? [HSDB]

Use the **limits** option of HSDB. Search for **leather tanning** in HSDB. Expand **Manufacturing/Use Information** and check the box for **Major Uses**. Click on several retrieved chemical records to view their “best sections” and click on **Human Health Effects** for these records in the Table of Contents.

7. Does nitrobenzene have any effect on sperm? Find some recent general articles on nitrobenzene. [HSDB, TOXLINE Core]

Search for **nitrobenzene sperm** in HSDB. Click on nitrobenzene record and view **Best Sections**. Click on **Other Files** and click on **TOXLINE Core**.

8. How does the U.S. Environmental Protection Agency characterize the carcinogenicity of methylmercury? [IRIS]

Search for **methylmercury** in IRIS and select the methylmercury record on the Search Results page. Expand category **II. Carcinogenicity Assessment for Lifetime Exposure**. Click on **II.A. Evidence for Human Carcinogenicity**.

9. Find any information on the occurrence or effects of methyl parathion in soil. Search using the chemical’s CAS Registry Number – 298-00-0. [HSDB]

Search HSDB for **298-00-0 soil** in the query box and scan the **Best Sections** of the methyl parathion record.

10. Use Boolean operators and phrase searching to look for information on lung cancer or mesothelioma in workers, in HSDB.

Enter – (“**lung cancer**” [htox] OR **mesothelioma** [htox]) AND **worker**

TOXNET Exercises (continued)

TOXICOLOGY LITERATURE FILES

1. Search TOXLINE Special for articles by C.N. Pope. Sort retrieval by primary author names. [TOXLINE Special]

Search for “pope cn” in query box. On “Search Results” page, click on “SORT” button and sort by author.

2. Search TOXLINE Special and TOXLINE Core for phosphoric acid. Explore navigating through your retrieval, examining individual records, and going to linked records. [TOXLINE Special & Core]

Search for **phosphoric acid** in query box. Make sure the **Both** radio button is selected. Click on **Details** buttons in both databases to view the respective search strategies. Navigate the pages. Click on records of interest and on hot-linked data – e.g. keywords, author names, CAS registry numbers. Check for related records.

3. Find articles focused on the effects of diet on breast cancer. [TOXLINE Special & Core]

Try a **Limits** search. Enter **diet breast cancer** in the query box. Limit to **Titles**. Select **Both** TOXLINE Special and TOXLINE Core.

4. Find journal references on the treatment of arthritis by the anti-inflammatory agent Celebrex. [TOXLINE Core]

Search for **arthritis celebrex** in the query box. Select the TOXLINE Core radio button.

5. Use the EMIC subfile to determine whether peppermint been tested for mutagenicity. Check for English language articles. [TOXLINE Special]

Conduct a Limits search. Select EMIC as a TOXLINE Component and English as a language from the drop down menus. Enter **peppermint** in the query box.

6. Find information on the effects of alcohol on the fetus. [DART Special and DART Core]

Select **Both** DART Special and DART CORE. Search for **alcohol fetus** in the query box.

TOXNET Exercises (continued)

7. Search TOXLINE Core directly on PubMed to find articles on toxicological aspects of jellyfish. Search for articles published from 2000-2002 in English. [TOXLINE Core via PubMed directly].

Go to PubMed at <http://pubmed.gov>. Click on **Limits**. Enter **jellyfish** in the search query box. Limit the search to the toxicology subfile, the publication dates to 2000-2002 and the language to English.

8. Find information on renal failure associated with amanita mushroom poisoning. Look for English language articles published from 1995 to 2002. [TOXLINE Special]

Conduct a Limits search. Enter **amanita renal failure** in the query box. Restrict publication years to 1995-2002. Select English from the dropdown menu.

9. Use the HISTORY feature to look for hospital or medical waste incineration in TOXLINE Special. [TOXLINE Special]

First search for **“hospital waste” incinerat***. (Using quotes looks for the terms together as a phrase. The asterisk is for truncation and searches for words such as incinerate, incineration, etc.) Then search for **“medical waste” incinerat***. Press the HISTORY button and combine your two searches according to the instructions, and using an “AND” operator.

TOXIC CHEMICAL RELEASES

1. How much ammonia was released to the air and water in Milwaukee in 1999?

In TRI99, search for **ammonia** in the “chemical name” query box and for **Milwaukee, WI** in the “facility location (city/state)” query box. Click on “Calculate Releases.”

2. How much of the above releases came from Red Star Yeast and in what body of water did this facility discharge ammonia?

After above search, go back to the “TRI Search Results” screen. Click on the Red Star Yeast record. Click on “Environmental Release of Chemical” in the Table of Contents. Scroll down to “Water Discharge Estimates.”

TOXNET Exercises (continued)

3. What chemicals have been released to the air, in amounts greater than 100,000 pounds, over Old Hickory, Tennessee in 1995 and 1996? By what companies?

Search for **Old Hickory Tennessee** in the “facility location (city/state)” query box. Select **greater than 100,000 pounds** for “total air release.” Results page will display chemicals and companies.

4. Did Hewlett-Packard’s Newark, California facility transfer any 1,2,4-trichlorobenzene off-site for treatment in 1996? How much? Where to?

In TRI96, search for **1,2,4-trichlorobenzene** in the “chemical” query box, **hewlett-packard** in the “facility name” query box, and **newark california** in the “facility location (city/state)” query box. Click on “Off-Site Waste Transfer” in the Table of Contents.

5. What company has reported the highest underground injection release of a single chemical in 1999? What was the chemical?

In TRI99, select **10,000,000** and “Total Underground Injection” in the “Greater than ___ for ___” drop down menus. For the records retrieved, expand the “Environmental Release of Chemical” category. Click on “Underground Injection Total” for these records and compare the numbers. Identify the chemical with the highest number.

6. How many individual TRI98 reports have been filed on barium compounds?

In TRI98, search **barium compounds** in the chemical query box. Note the number of records retrieved listed at the top of the Search Results page.

HAZ-MAP

1. What are some high risk tasks associated with the job of carpet installation?

Click on **High Risk Jobs** and then on **Carpet Installers**.

TOXNET Exercises (continued)

2. What are some hazards associated with the use of cobalt in the workplace?

Click on **Hazardous Agents**, then on **Cobalt**. Click on **Cobalt** again to view exposure assessment data. Extra – from here highlight some terms and press Search **TOXLINE** to perform a TOXLINE search.

3. What are some hazards of leather tanning?

Perform a “text search” for **leather tanning** in the search query box. Click on **leather tanning and finishing** as an Industry and **tanning leather** as a Process.

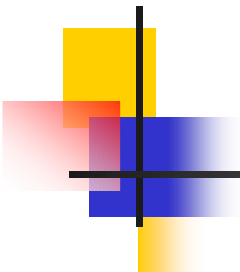
WORLD WIDE WEB

1. Explore EPA’s voluminous Web site, particularly the **Databases and Software** section located by clicking on their home page’s **Information Sources**. Locate IRIS, ECOTOX, the Toxics Release Inventory, and the Safe Drinking Water Information System. Use the Advanced Query box to find documents with **mercury** in the title. [www.epa.gov]
2. Locate a full-text article on why drugs get pulled off the market in the January-February 2002 issue of the **FDA Consumer** magazine. [www.fda.gov]
3. What chemicals are on the list of “Known to be Human Carcinogens” in the National Toxicology Program’s Year 2000 9th Annual Report of Carcinogens? [ntp-server.niehs.nih.gov]
4. Find the Agency for Toxic Substances and Disease Registry’s TOXFAQ profile on nickel. [www.atsdr.cdc.gov]
5. Check out the National Council for Science and the Environment’s Web site and find recent Congressional Research Service (CRS) reports on **pesticides**. [www.cnie.org]
6. Which Florida universities offer graduate programs in toxicology? Check the Society of Toxicology’s Resource Guide to Careers in Toxicology (under Public Outreach/Career Resources) [www.toxicology.org]

TOXNET Exercises (continued)

7. Explore the variety of data sources containing information on acrylonitrile, by searching ChemFinder. [www.chemfinder.com]
8. Where and on what dates will the Society of Environmental Toxicology and Chemistry's 2003 Annual Meeting in Europe be held? [www.setac.org]
9. What is New Jersey's rank among states in total release hazardous air pollutants? Use Scorecard (from Environmental Defense). Start by clicking on Hazardous Air Pollutants. View the New Jersey Report, particularly the Ranking by Health Risks section. [www.scorecard.org]
10. How many poison control centers in Texas are certified by the American Association of Poison Control Centers (AAPCC)? What are their phone numbers? The AAPCC's Poison Center Lists includes a list of certified centers. [www.aapcc.org]
11. Use the BIOLOG file (one of Syracuse Research Corporation's Environmental Fate Data Bases - EFDB) to find information about DDT in sewage. [esc.syrres.com]
12. Use the Environmental Journalism site to determine what environmental meetings will be coming up in December 2002. [www.sej.org]
13. How do Health Canada, the U.S. EPA, and ATSDR's evaluations of the noncancer inhalation risk values of styrene compare? [www.tera.org/iter]
14. What are some common side effects of the drug, Vioxx? Consult MEDLINEplus' Drug Information page (data from the USP). [www.nlm.nih.gov/medlineplus/druginformation.html] .

Also consider RxList [www.rxlist.com].
15. Who makes Kill Zone Flea and Tick Killer 2000? What are its active ingredients? How have various governmental agencies rated the carcinogenic potential of these ingredients? [www.pesticideinfo.org]



Part VI

ChemID*plus*

- Chemical Identification File
- Chemical Dictionary/Directory File for chemicals cited in MEDLARS Files & outside resources
- Contains over 350,000 chemical records
- Structural Data for over 110,000 records
- Direct Link/Searches of MEDLINE, TOXNET, and other resources



ChemID*plus* Content

Names and Synonyms

- **Name of Substance**: Usually the most commonly used name, includes MeSH heading and USAN name
- **MeSH Heading**: NLM Medical Subject Heading
- **Systematic Name**: Describes molecular structure
- **Synonyms**: All other names found for the substance
- **Mixture Name**: Name of multi-component substance, one of which is the retrieved substance
- **SUPERLIST names**: The name used by regulatory/guidance lists



ChemID*plus* Content

- **CAS Registry Number**: Unique number of up to 9 digits assigned by Chemical Abstracts Service used to index chemicals. ChemIDplus uses the hyphenated format
- **ID**: The ID number is the CAS Registry Number in a non-hyphenated fixed length format or a unique number for entries that have no CAS Registry or NLM assigned numbers
- **Molecular Structure**: Display of structure (if present) via Chime or ChemSymphony
- **Registry Numbers**: All CAS Registry Numbers known to be assigned over time to a specific compound



ChemID*plus* Content

- **Formulas**: The molecular formula in a hyphenated format.
- **Classification Codes**: Describe the general category assigned by a given source to a chemical based on toxicity, use and application, pharmacologic and/or therapeutic category, and status on certain chemical lists.
- **Notes**: A textual description of a compound's use and utility, often from MeSH controlled vocabulary.
- **Locators**: The names of NLM databases, and other major resources that have information about a given compound, usually hyperlinked.

Division of Specialized Information
Services, NLM
ChemID_{plus} Chemical Search Input
Page
A TOXNET Resource

Welcome to a new
and improved
version of
ChemIDplus!



ChemIDplus

352827 Records

117102 Structures

Powered by Chemscape™

<http://www.mdli.com/chemscape>

Data Search Type:

Name/Synonym	Definition	Prevalence	Pathogenesis	Diagnosis	Management
<p>Chronic obstructive pulmonary disease (COPD)</p> <p>Chronic bronchitis</p> <p>Emphysema</p>	<p>Chronic inflammation of the airways and lung tissue, leading to airflow limitation.</p> <p>Chronic inflammation of the bronchi, leading to mucus production and airway narrowing.</p> <p>Abnormal enlargement of the alveoli, leading to loss of lung elasticity and impaired gas exchange.</p>	<p>~10-15% in the US, ~10% in the UK.</p> <p>~10-15% in the US, ~10% in the UK.</p> <p>~10-15% in the US, ~10% in the UK.</p>	<p>Long-term exposure to cigarette smoke, air pollution, and occupational dusts.</p> <p>Genetic factors (e.g., alpha-1 antitrypsin deficiency).</p> <p>Chronic inflammation and destruction of lung tissue.</p>	<p>History and physical examination, chest X-ray, spirometry.</p> <p>History and physical examination, chest X-ray, spirometry.</p> <p>History and physical examination, chest X-ray, spirometry.</p>	<p>Smoking cessation, inhaled corticosteroids, long-acting beta-agonists, oxygen therapy.</p> <p>Smoking cessation, inhaled corticosteroids, long-acting beta-agonists.</p> <p>Oxygen therapy, lung volume reduction surgery.</p>

Equals

MTBE

And optional Locator Code limit is

Please choose one

Structure Input Box



Structure Search Type: Substructure Search ▼

Display 10 Results

Display chemical structures using

Chime 

Change Now

Java 6

Search

Clear

Help

[Chemical Information Home Page](#)

[SIS Home Page](#)

[TOXNET Home Page](#)

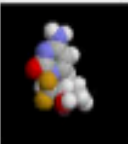
Structure WebMaster




ChemID*plus* Search Screen

Five drop down menus on the search screen:

- Data Search Type: Names/Synonym, Registry Number, Formula (hyphenated), Classification Code, Locator Code
- Logical Operators: Equals (the default), Starts With, Contains
- Display results: 10 (default), 25
- Locator Code (optional limit): List of files and locators, MEDLINE, TOXLINE, EPA, FDA, WHO, OSHA, CDC
- Structure Search Type: Substructure Search, Similarity Search (default 80% similarity), Exact Structure



Methyl tert-butyl ether RN: 1634-04-4



[Enlarge Structure](#)

Molecular Structure

Names and Synonyms

Classification Codes

Formulas

Notes


















Registry Numbers

Locator Codes

Entire Record

Main Query Page

File Locator

-  [CANCERLIT](#)
-  [CCRIS](#)
-  [DART/ETIC](#)
-  [DSL](#)
-  [EINECS](#)
-  [EMIC](#)
-  [HSDB](#)
-  [IRIS](#)
-  [MEDLINE](#)
-  [MEDLINEplus](#)
-  [MESH](#)
-  [RTECS](#)
-  [SUPERLIST](#)
-  [TOXLINE](#)
-  [TRI95](#)
-  [TRI96](#)
-  [TRI97](#)
-  [TRI98](#)
-  [TRI99](#)
-  [TSCAINV](#)

Welcome to the ChemIDplus Locator Page

The window to the left displays one or more ChemIDplus Locator Codes which link to other sites that carry information about the chemical you have retrieved. **You may click on:**

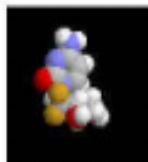
- A hyperlinked Locator Code such as [TOXLINE](#) to retrieve data from that resource. Results will be displayed in this window.
- The information icon () to get a description of the source of the Locator Code and the scope of the search.

The window on the top of the screen displays buttons that you may click on to change the data displayed for this chemical or to change your search mode. Hold your mouse pointer over a button to see a more detailed description.



Locator Code Page

- Hyperlinked locators directly search resources on a substance
- Information icon (i) next to the locator gives the description of the database and scope




Query Results 1 - 2 of 2

Main Query
Page

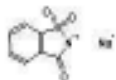
ChemIDplus

Options	ID	Structure	CAS	Molecule Name	Formula
Full Record Enlarge Structure Use Structure For Query Use Structure for Similarity	000081072		81-07-2	Saccharin [USAN]	C7-H5-N-O3-S
Full Record Enlarge Structure Use Structure For Query Use Structure for Similarity	000128449		128-44-9	Saccharin sodium anhydrous	C7-H5-N-O3-S.Na



ChemIDplus

Saccharin sodium anhydrous RN: 128-44-9



[Enlarge Structure](#)

Molecular Structure

Names and Synonyms

Classification Codes

Formulas

Registry Numbers











Locator Codes

Entire Record








Search Results Page

Main Query Page

File Locator


-  [CCRIS](#)
-  [DART/ETIC](#)
-  [DSL](#)
-  [EINECS](#)
-  [EMIC](#)
-  [GENETOX](#)
-  [RTECS](#)
-  [SUPERLIST](#)
-  [TOXLINE](#)
-  [TSCAINV](#)

Superlist Locator

-  [CA63](#)
-  [HPV](#)
-  [IARC](#)
-  [INER](#)
-  [MA](#)
-  [PA](#)
-  [PAFA](#)

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Zidovudine [USAN:BAN:INN:JAN] RN: 30516-87-1

Molecular
Structure

Names and
Synonyms

Classification
Codes

Formulas

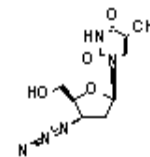
Notes

Registry
Numbers

Locator
Codes

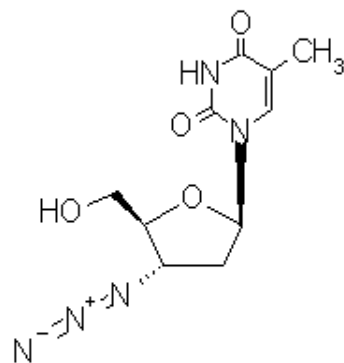
Entire
Record

Main Query
Page



[Enlarge Structure](#)

[ChemIDplus](#)



ID:
030516871

CAS Number:
30516-87-1

Enlarge
Structure

Use Structure
For Query

Use Structure
for Similarity

Formula:
C10-H13-N5-O4

**Names and
Synonyms**

MeSH Heading

• Zidovudine

Name of Substance

• Zidovudine
• Zidovudine [USAN:BAN:INN:JAN]

Superlist Name

- 1-(3-Azido-2,3-dideoxy-beta-D-ribofuranosyl)-5-methylpyrimidine-2,4-(1H,3H)-dione
- 3'-Azido-3'-deoxythymidine
- Zidovudine

Synonyms

- (component of) Combivir
- (component of) Trizivir
- 3'-Azido-3'-deoxythymidine
- AZT
- Azidothymidine
- BW A509U
- BW-A 509U
- CCRIS 105
- Compound S
- DRG-0004
- HSDB 6515
- NSC 602670
- Retrovir
- Zidovudina [Spanish]
- Zidovudine
- Zidovudinum [Latin]

Systematic Name

- Azidothymidine
- Thymidine, 3'-azido-3'-deoxy-

**Classification
Codes**

Classification Code

- Anti-HIV agents
- Antimetabolites
- Antimetabolites, antineoplastic
- Antiretroviral
- Antiviral
- Drug / Therapeutic Agent
- Human Data
- Mutation data
- Reproductive Effect
- Reverse transcriptase inhibitors
- Tumor data

Superlist Classification Code

- Overall Carcinogenic Evaluation: 2B

Formulas

Molecular Formula

- C10-H13-N5-O4

Locators

File Locator

- AIDSDRUGS
- AIDSLINE
- CANCERLIT
- CCRIS
- DART/ETIC
- DSL
- EMIC

- HSDB
- MEDLINE
- MEDLINEplus
- MESH
- MESH HEADING
- RTECS
- SUPERLIST
- TOXLINE

Internet Locators

- NIAID HIV DRUGS
- healthfinder

Superlist Locator

- IARC
- NTPT

Notes

Note

• A dideoxynucleoside compound in which the 3'-hydroxy group on the sugar moiety has been replaced by an azido group. This modification prevents the formation of phosphodiester linkages which are needed for the completion of nucleic acid chains. The compound is a potent inhibitor of HIV replication, acting as a chain-terminator of viral DNA during reverse transcription. It improves immunologic function, partially reverses the HIV-induced neurological dysfunction, and improves certain other clinical abnormalities associated with AIDS. Its principal toxic effect is dose-dependent suppression of bone marrow, resulting in anemia and leukopenia.

Registry Numbers

CAS Registry Number

- 30516-87-1



ChemID*plus* Exercises

1. Check the file locator to see what NLM databases contain information on phenytoin. Search DART without leaving ChemID*plus*.

Type Phenytoin in search box, click Search. Click DART/ETIC in left pane under File Locator, view record in right pane.

2. Locate the record for styrene and link to the Internet Locator ATSDR TOXFAQS. Next link to the NIOSH Pocket Guide. Is styrene on the EPA Clean Air Act (CAA1)? Activate the Classification Code button and find the IARC classification on carcinogenicity, click on the "i" to see the source.

Type styrene in the search box, click Search. Scroll down the left pane and under Internet Locators click the link to ATSDR TOXFAQs. Next, scroll down and under Superlist Locator click the link to the CAA1 listing for styrene. At the top of the screen, click the button for Classification Code. Under Superlist Classification Code, click the "i" for Overall Carcinogenic Evaluation..... to view this source in the right pane.

3. Find the "valium" record in ChemID*plus* and use its structure to do substructure and similarity searches respectively. How many structures are in each category?

Type valium in the search box, click Search. Now click the Molecular Structure button at the top. Click Use Structure for Query button. Choose Similarity Search from the Structure Search Type pull-down list and click Search. Type in a percent similarity between 50 and 100, the default is 80 percent, but you may have to use a lower number if you don't retrieve any hits. For a substructure search, go back to the Structure Search page (click back button on your browser), choose Substructure Search from the Structure Search Type pull-down list, click Search

4. Identify all the HSDB records that are ozone depletors (CAA2).

Choose Locator Code from the Data Search Type pull-down list. Type HSDB in the search box. In the pull-down list that says "and optional Locator Code limit is" choose CAA2 from the pull-down list. Click Search.